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PREDICTING FLOW IN ALUMINA DIGESTION VESSELS

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ABSTRACT

Single-phase computational studies of two different digester vessel designs, carried out circa 2005, gave results that did not compare well with the associated laboratory-scale experimental measurements for all configurations. With the continued development of commercially-available computational fluid dynamics software, it was decided to revisit the predictions for both vessel designs, using ANSYS CFX 15.0. Transient models were studied to investigate the impacts of a variety of turbulence models, along with the effects of mesh quality/refinement. The chief focus of the research program was the efficacy of a variety of turbulence models - Two-equation (k-ε, SST), Reynolds Stress (SSG RSM) and Scale Adaptive Simulation (SAS-SST) were all considered. The predicted velocity profiles are compared with high quality Laser Doppler Velocimetry (LDV) data. The calculated residence times are compared with salt tracer estimates from experiments. The importance of small-scale turbulence structures in determining the flow profile and residence times of the vessels is highlighted in this study.

INTRODUCTION

Digestion plays a fundamental part in the Bayer process for alumina production, with the objective of this processing stage being to extract the available alumina from the bauxite by dissolving it in a hot caustic soda solution. Digester vessels typically have a height to diameter ratio of close to 3:1. Some vessels use mechanical agitation, but those examined in this study have a single inlet stream at the top of the vessel and a single, centrally located, outlet at the bottom of the vessel, as in the schematic shown in Fig. 1. The flow behaviour in these vessels is therefore dominated by the design and positioning of the inlet nozzle. An understanding of the flow behaviour in these vessels is important as adequate residence time and mixing are critical to achieving sufficient extraction of alumina from bauxite particles of varying diameter.

Past modelling within the organisation used k-ε, in steady-state simulations (Brown and Fletcher, 2005). While the simulations of top-fed digesters were considered to give acceptable agreement with experiment, the same could not be said for the simulations for tangentially fed vessels.

Woloshyn, Oshinowo and Rosten (2006) used CFD to investigate a range of digester feed configurations. This study considered full-scale digesters using the k-ε and Reynold Stress Model for turbulence. Residence Time Distributions (RTD) were determined for individual particles of various sizes. However, no validation of the simulations was conducted.

Brown, Whyte and Fletcher (2014) studied the flow in precipitation vessels using CFD. These vessels have comparable flow rates and velocity scales as the digesters. The work evaluated a variety of turbulence models and validated the numerical predictions against experimental measurements. The authors found that using a turbulence model that was able to capture the underlying local velocity fluctuations gave results that matched the experimental data very well.

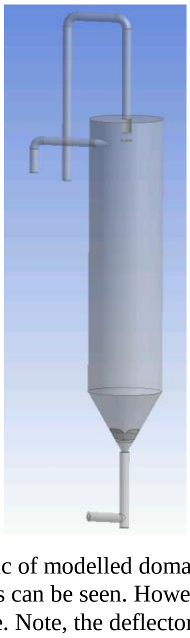

Figure 1: Schematic of modelled domain. Both top and tangential feed lines can be seen. However, only one feed is active at any time. Note, the deflector plate suspended below the top feed nozzle which stops flow from short-circuiting to the outlet.

Thus, given improved modelling techniques and computational resources, it seemed appropriate to revisit the modelling of the digesters. Below, we give a brief description of the experimental study used for validation purposes and then compare simulation results with the experimental data, first for the top-fed vessel and then for the vessel with a tangential inlet.

EXPERIMENTAL STUDY

Alcoa commissioned CSIRO Minerals Resources Flagship to provide the experimental data used in this study. A laboratory-scale (~1.5 m tall and diameter of ~0.4 m) model of a full-scale digester was used in the experiments. Water was used as the working fluid. The data reported here are for an inlet flow rate of 127 l/min.

Superficial residence time, is a crude estimate of how long a particle will be present within a vessel, and is defined as the volume of the domain divided by the flow rate through the domain. In the cases being considered here, the superficial residence time, T_o, is ~88 s. The results of experiment and simulation will be compared over a normalised time (measured time, t, divided by T_o).

Laser Doppler Velocimetry (LDV) was used to measure the velocity components along a line from the central axis to just off the vessel walls. These readings were taken at several vertical elevations – those taken at 415 mm and 1465 mm above the cone are reported here. The measurement device is held stationary at each point along the radius for approximately two minutes, with 2000 readings taken in each period.

Residence Time Distributions (RTD) were determined using a salt tracer. A pulse of salt was injected into the inlet pipe and the concentration of salt was measured at the outlet over time.

MODEL DESCRIPTION

Turbulence Modelling

Different turbulence modelling approaches were tested in an effort to determine the most accurate method for calculating the flow field, whilst balancing computational requirements. As flow separation is not a governing feature of the flow, wall functions are considered to be sufficient to predict flow in the wall region.

Previous work had shown that k-ε (Launder and Spalding, 1974) could predict the flow of the top-fed digester but was lacking in prediction of behaviour in the tangentially fed devices. The k-ε model resulted in steady-state behaviour, where the experiments indicated a certain amount of unsteadiness. The two-equation SST (Menter, 1994) and Reynolds Stress Model (SSG RSM) (Speziale, Sarkar and Gatski, 1991) were also tested. Finally, given the success in predicting unsteady flow in lab-scale precipitators (Brown, Whyte and Fletcher, 2014), the Scale Adaptive Simulation (SAS-SST) was considered (Menter and Egorov, 2010). When applying the SAS-SST model the local turbulence structures are captured if the mesh is fine enough and the flow is globally unsteady. If it is not the simulation model may remain in SST mode. In order to avoid this, a zonal LES region was introduced in the inlet feed pipe in order to convert modelled turbulence into resolved turbulence and ensure that the SST-SAS model behaved in SAS mode.

Computational Domain and Mesh

The meshes used in this study were informed by the experience in modelling alumina precipitators (Brown, Whyte and Fletcher, 2014). The tangentially-fed digester is inherently 3-dimensional, so no attempt was made to reduce the geometrical complexity.

Experience has shown that for systems such as those discussed here, a good starting point for mesh inflation is, 10 layers of inflation on all walls with a 1 mm first layer height and 1.2 expansion ratio. In subsequent meshes, these controls were changed to 20 layers, with a first layer of 0.5 mm. This gave y^+ values typically in the range of 20-30. General guidelines for an appropriate mesh density for the SST-SAS model in this sort of geometry are not available, with the majority of published cases being related to bluff body or aerodynamic flows. Therefore, the edge length of the mesh in the main vessel was systematically reduced and the results assessed. The meshes used are shown in Figure 2.

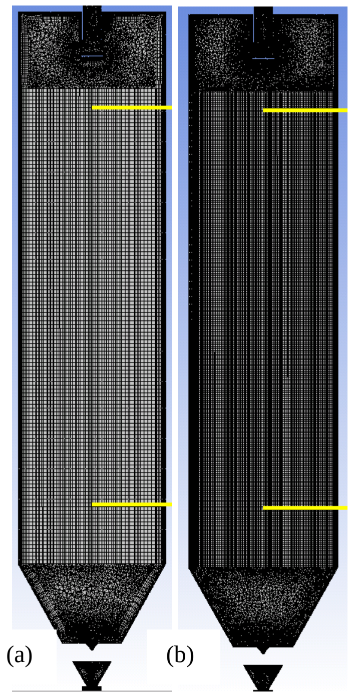

Figure 2: Representations of the computational meshes used in the study. The inlet region and lower cone were meshed using tetrahedrons, while the barrel of the digester was swept. (a) This mesh has ~610,000 nodes, with a first inflation layer height of 1.0 mm; (b) this mesh has ~2,700,000 nodes, with a first inflation height 0.5 mm. The yellow lines represent the 415 mm (lower) and 1465 mm (upper) elevations used for comparison with experiments.

Numerical Considerations

The commercial CFD code ANSYS CFX 15.0 was used for this study. The code uses a vertex-based control volume approach; uses the Rhie-Chow procedure to couple pressure and velocity; and an algebraic multi-grid solver to solve the equations of motion. Spatial and temporal derivatives were calculated using second order bounded differencing schemes.

All simulations were carried out as transients and run for 300 s (~3 superficial residence times). Simulations that evolved to a steady-state were terminated prior to reaching the target time. The transient simulations were specified with adaptive time-stepping – SAS-SST simulation typically requiring time steps of ~10^{-3} s, and two-equation models reached the upper limit of 0.1 s.

RESULTS

In this section we will focus on the comparison of the k-ε and SAS-SST turbulence models. While the SST and SSG RSM models were considered in the study, neither provided better predictions of the experiments (or offered additional insight) than k-ε or SAS-SST. It is interesting to note that in both inlet configurations, the k-ε models resulted in effectively steady velocity fields (fluctuations <<0.1% of the mean flow) on both the fine and coarse meshes.

The results presented here were obtained from a set of calculations carried out to determine the expected Residence Time Distribution (RTD) curves for the vessels. An additional mass-less tracer field was included in the models and the concentration at the vessel outlet was monitored (Brown, 2001). In the case of the k-ε models, the fluid was treated as a *frozen* velocity field. While, in simulations using the SAS-SST model, the flow was allowed to freely evolve. Statistics of the transient flow are taken over the whole simulation period – the following plots show the time-averaged values of various variables. In both the SAS-SST predictions and LDV measurements, the standard deviation of the components of velocity have been used to indicate the magnitude of flow fluctuations.

An effective approach to detecting vortex structures is the second invariant of the velocity gradient tensor (or *Q*-criterion) (Hunt, 1987),

$$Q = \frac{1}{2}\left(|\Omega|^2 - |S|^2\right),$$

where Ω and S are the vorticity and shear strain rate tensors, respectively. Vortical structures can be identified by isosurfaces for $Q > 0$.

Top fed digester

The predictions for the top fed digester show good agreement with experimental data, almost regardless of the turbulence model used. The vertical component of velocity is the dominant flow direction in this configuration. In Figure 3 we can see the similarity of the predictions of the k-ε and SAS-SST turbulence models – where the key difference is the extent of a recirculation zone under the deflector plate. Both turbulence models predict very similar vertical velocity profiles but show some disagreement with experimental values near the walls under the deflector plate, and uniform down-flow in the lower half of the vessel (Fig. 4). There is a significant difference in the flow structure predicted by the two models, as expected. An additional point of agreement between the measurement from LDV and SAS-SST predictions, is the magnitude of the fluctuations seen in the velocity components (Fig. 4).

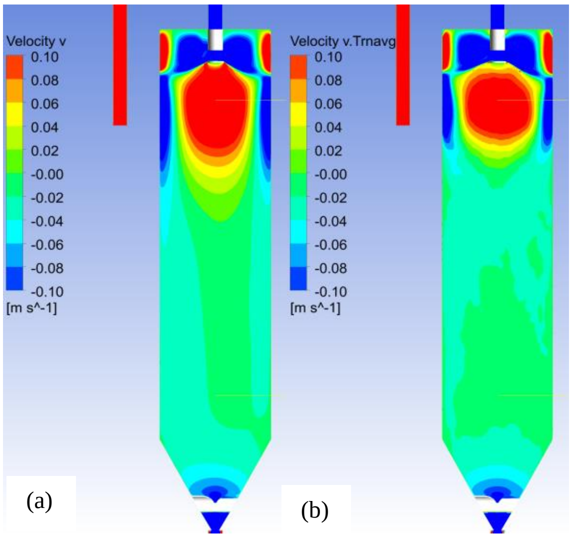

Figure 3: Contours of the vertical component of fluid velocity (negative values indicate down-flow). (a) k-ε, on the coarse mesh; (b) SAS-SST, on the fine mesh. In both cases, the flow features show qualitative similarities. There is strong down-flow at the wall below the deflector plate. Directly under the deflector plate is a region of strong recirculation – there is a slight difference between the two predictions. However, beneath this region there is fairly uniform down-flow.

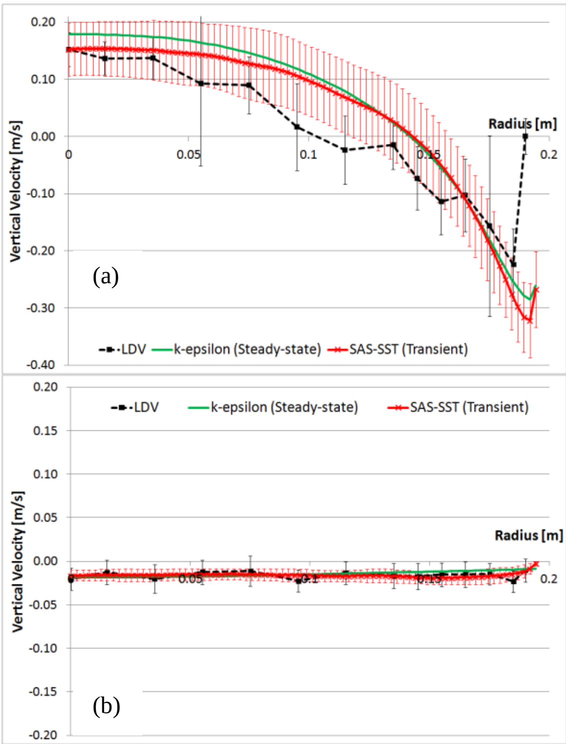

Figure 4: Comparison of predicted vertical components of velocity with LDV measurements - (a) taken along the radius of the vessel at 1465 mm; (b) at 415 mm. Both models predict the same general behaviour. In (a) there is upflow on the central axis (beneath the deflector plate), with faster down-flow at the walls; (b) shows a relatively slow, uniform down-flow in the lower part of the vessel. It should also be noted that the magnitude of the fluctuations of the SAS-SST predictions and LDV measurements are similar.

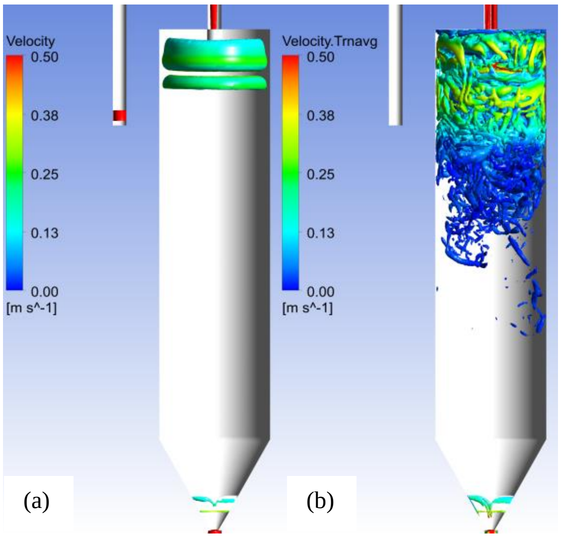

Figure 5: Isosurface of Q-criterion=10 s^{-2}, coloured by velocity. (a) k-ε, on the coarse mesh; (b) SAS-SST, on the fine mesh. In (a) we can observe that the 2-equation model only captures the structure of the upper recircuation caused by the deflector plate; (b) highlights the siginificant amount of turbulence structure resolved by SAS-SST in the upper region of the chamber. The deflector plate generates turbulence in the flow, that then dissipates in the lower regions of the digester.

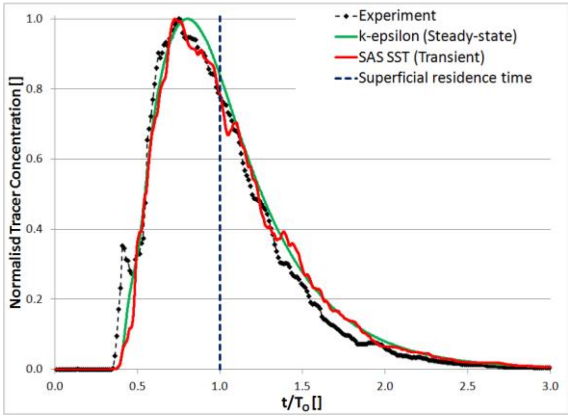

Figure 6: RTD curves for predicted flows and experimental measurement. There is very little difference in the tracer peaks. Interestingly, the curves are very similar for both the k-ε frozen fluid (steady-state flow field) and the transient SAS-SST prediction. Previous modelling within our organisation also found this to be the case (Brown and Fletcher, 2005). In some sense, the top feed digester appears to be less sensitive to the fine detail of the flow field.

Figure 5 shows that the flow predicted by the k-ε model is dominated by the recirculation produced by the deflector plate, while the SAS-SST flow has a significant amount of structure in the upper section of the vessel. However, the RTD curves (Fig. 6) suggest that these fluctuations have very little impact on fluid retention times.

Tangentially Fed Digester

It is the models of tangentially fed digesters that are most interesting here, as past efforts show that two-equation models were insufficient to accurately predict the flow field or fluid retention times. In this case we are interested in the vertical and tangential components of the flow.

Figure 7 illustrates that the predicted vertical velocity fields, while showing global similarity, have some significant local differences. In particular, the down-flow seen in the central axis is more extensive in the k-ε model. In Fig. 8, we can see that neither of the models predicts the magnitude of the central up-flow shown by the LDV data. Figures 9 and 10 show that both models predict the swirling flow profile with SAS-SST being clearly superior.

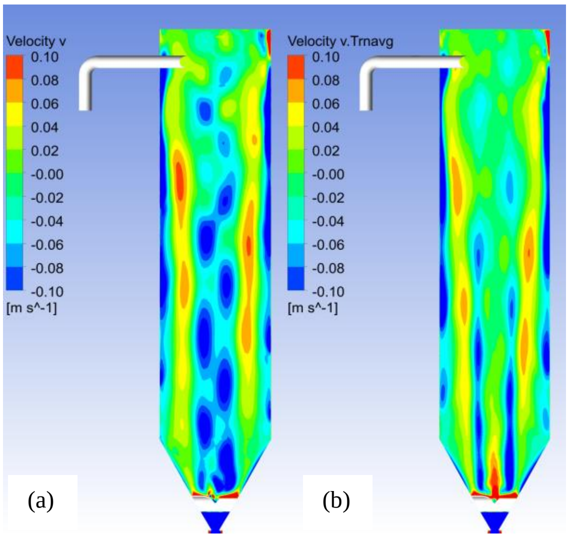

Figure 7: Contours of the vertical component of fluid velocity. (a) k-ε, on the coarse mesh of Figure 2(a); (b) SAS-SST, on the fine mesh of Figure 2(b). While there are some qualitative similarities between the two cases, the differences are quite clear – the two-equation model predicts that the down-flow region of the central core extends to the full height of the vessel, and the flow is more *erratic*.

Considering the turbulence structure evident in the predictions of the SAS-SST model (Fig. 11) as indicators of the presence of significant fluctuations in the velocity field, we can examine the extent of error in the mean flow predictions. In Figure 10, we can see that there is overlap of the fluctuating aspects of experimental and modelled flow fields. It is clear that a steady-state flow field is in error here. This is further supported by examination of the RTD curves shown in Figure 12. The effectively steady-state solution predicted using the k-ε model does not replicate the experimental RTD curve – the curve is somewhat too steep and the peak in tracer concentration at the outlet occurs later (~20% longer than experiment). On the other hand, the RTD curve predicted by the transient SAS-SST model under-predicts the time of the peak in outlet tracer concentration by approximately 20%, while the general form of the curve is very similar to the experimental result. The SAS-SST model does not capture the full extent of the back mixing region evident in the experiments (note the up-flow in Fig. 8(b)). This suggests an important role played by accurate representation of local velocity fluctuations in the global performance characteristics of the vessel. In our industrial setting, this k-ε model may just be sufficient for evaluation of technology.

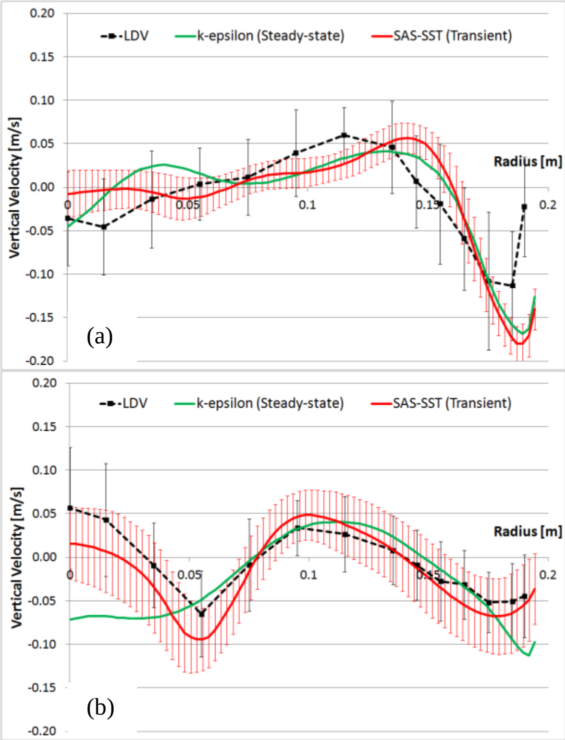

Figure 8: Comparison of predicted vertical components of velocity with LDV measurements. (a) taken along the radius of the vessel at 1465 mm; (b) at 415 mm. In (a) we can see that all models are quite consistent, and neither predict the flow profile at the wall accurately; (b) highlights that the key difference between models is the ability to predict the upflow on the centre-line in the lower region of the digester – only the SAS-SST model is partially successful in predicting this behaviour.

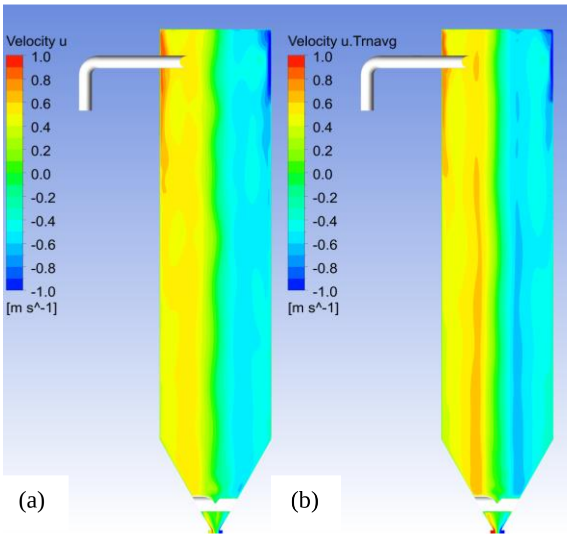

Figure 9: Contours of the tangential component of fluid velocity. (a) k-ε, on the coarse mesh; (b) SAS-SST, on the fine mesh. There is very little difference between the predictions of the two models.

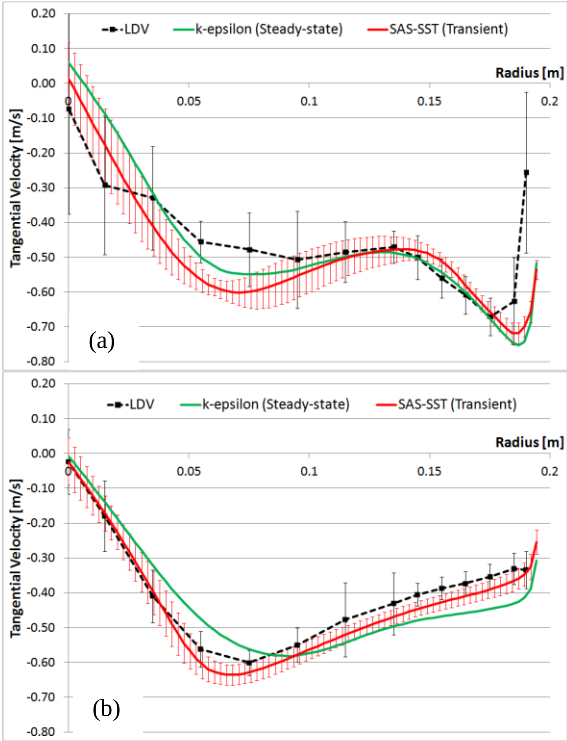

Figure 10: Comparison of predicted tangential components of velocity with LDV measurements. (a) taken along the radius of the vessel at 1465 mm; (b) at 415 mm. Both plots show that the SAS-SST model provides the most accurate prediction of the velocity profile.

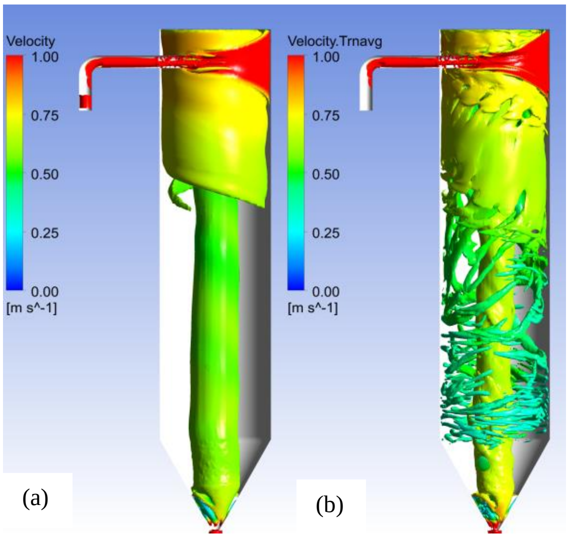

Figure 11: Isosurface of *Q*-criterion=10 s^{-2}, coloured by velocity. (a) k-ε, on the coarse mesh; (b) SAS-SST, on the fine mesh. In (a) we see that the k-ε captures the bulk swirl structure, while in (b) the resolved turbulence structure exists on top of this swirl, and does not dissipate as in the top-fed digester (see Figure 5(b)).

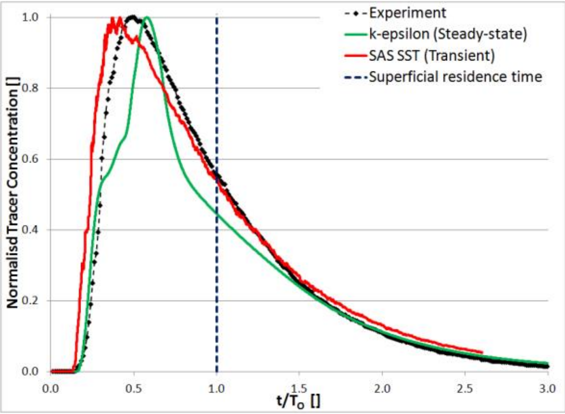

Figure 12: RTD curves for predicted flows and experimental measurement. Neither model returns an RTD curve that matches the experiment as well as the predictions for the top-fed configuration. The SAS-SST based prediction does capture the general shape of the experimental data but estimates that the peak in tracer concentration at the oulet occurs sooner than in the experiment.

CONCLUSION

We have shown that an accurate model for top fed digesters has been developed. Within the limit of the cases studied, the simulated flow in the top-fed digesters is independent of turbulence models used. The agreement between RTD predictions of steady-state and transient models, with experimental data, suggests that in this feed orientation, the fine detail of turbulence is not important in predicting the performance of the vessel.

However, to predict the flow field and residence time of the tangentially-fed digester, it appears that faithful prediction of the small-scale turbulence structure is essential. All models gave reasonable predictions of the swirl profile. The key difference is seen in the vertical velocity component of the flow – the experimental results shows up-flow on the centre-line in the lower regions of the vessel. The SAS-SST model was the only turbulence model that went some way to replicating this behaviour. While the SAS-SST model displayed greatly improved predictions of the experimental velocity profile, the RTD was under-predicted, which indicates that there are further flow features that remain undetermined. It should also be noted that using SAS-SST for modelling a production scale digester may prove computationally prohibitive.

The next-step in model development is to use a multiphase model to enable study of size specific particle retention times.

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REFERENCES

BROWN, G.J. and FLETCHER, D.F., (2005), Aloca internal report, October 2005.

BROWN, G.J., (2001), "CFD Prediction of Particle and Fluid Residence Times in Industrial Vessels", *6th World Congress of Chemical Engineering*, Melbourne, Australia.

BROWN, G.J., WHYTE, D.S., and FLETCHER, D.F., (2014), "Dynamic flow modelling in precipitator vessels – A study of turbulence modelling approaches", *Appl. Math. Model.*, **28**, 4163-4174.

HUNT, J.C.R., (1987), "Vorticity and vortex dynamics in complex turbulent flows", *Transactions of the Canadian Society for Mechanical Engineering*, **11** (1), 21–35.

LAUNDER, B.E. and SPALDING, D.B., (1974), "The numerical computation of turbulent flows", *Comp. Meth. Appl. Mech. Eng*., **3**, 269-289.

MENTER, F.R., (1994), "Two-equation eddy-viscosity turbulence models for engineering applications", *AIAA J*., **32**(8), 1598-1605.

MENTER, F.R and EGOROV, Y., (2010), "The Scale-Adaptive Simulation method for unsteady turbulent flow predictions. Part 1: Theory and model description", *Flow Turbulence Combust*. **85**, 113–138.

SPEZIALE, C.G., SARKAR, S. and GATSKI, T.B., (1991), "Modelling the pressure-strain correlation of turbulence: an invariant dynamical systems approach", *J. Fluid Mech.*, **277**, 245-272.

WOLOSHYN, J., OSHINOWO, L., and ROSTEN, J., (2006), "Digester Design Using CFD", *135th Annual Meeting - Proceedings of the Technical Sessions presented by the TMS Aluminium Committee*, 939-944.